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Assessment of Tools for Molten Salt Reactor Dose Rate Calculations

Nuclear Science and Engineering Division

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prepared by
Yan Cao and Bo Feng
Nuclear Science and Engineering Division, Argonne National Laboratory

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Abstract

This report discusses a preliminary assessment of the capabilities of current state-of-the-art stochastic codes Shift and MCNP6 to calculate the ex-core radiation dose rates for a simplified Molten Salt Reactor (MSR) model. The Monte Carlo code Shift has been under significant development in recent years at ORNL as part of the CASL program and is now supported by NEAMS. Originally, Shift was developed for LWR ex-core calculations but with dose rate and shielding calculations specifically requested by the NEAMS program's MSR industry partners, the MSR Application Drivers team was tasked with assessing Shift for non-LWR applications. This was the first application of the Shift code for non-LWRs and the findings can be considered preliminary due to the activities occurring only over a 5-month period. Attractive features of Shift include massive parallelization and advanced automated variance reduction techniques such as CADIS and FW-CADIS.

To provide a basis of comparison, the non-NEAMS Monte Carlo code MCNP6 was also used to calculate the radiation dose rates for a simplified MSR shielding test problem. ANL and ORNL contributors to this MSR Application Drivers activity worked together to set up and run the Shift code successfully on the INL HPC cluster. A second goal of this work was to build Shift user experience at ANL for future applications such as performing shielding analysis for a more detailed and publically available MSR design such as the Molten Salt Breeder Reactor (MSBR). The ANL analysts successfully applied both the MCNP6 and Shift codes to calculate radiation dose rates at places far away from the core where neutron fluxes are attenuated by more than 10^{14}. The variance reduction techniques such as the weight window are important and enable both codes to transport particles through the thick shield. The key differences of generating the weight windows for both codes are discussed in this study.

1 Introduction

This work was performed under the DOE-NE NEAMS work package MSR Application Drivers to leverage the existing and developing capabilities of NEAMS tools bridging gaps in the MSR M&S field. The main scope of the current work in fiscal year 2020 is to assess the capabilities of current numerical tools, including both NEAMS numerical codes and non-NEAMS codes to calculate the radiation dose rates for future MSR reactors.

The PROTEUS-SN neutronics code developed under the DOE-NE NEAMs program was first used to model the simplified MSR core model used in this study. These shielding calculations were performed as a response to interest from industry on NEAMS capabilities to perform such assessments. Numerical analyses demonstrated the capabilities of the code for calculating critical eigenvalues of the core, power distribution maps within the core, and temperature feedback coefficients [1]. However, for dose rate calculations outside of the core zone, where neutron particles would have had to penetrate through thick shielding layers, the PROTEUS-SN results generated from the scoping study were not deemed adequate for those needs. This was expected as this approach is dependent on the number of energy groups, spatial meshes, and angular direction points and its order of Legendre expansions used in the model. The inadequate coarse mesh adopted may also have caused negative fluxes. For designs with large non-scattering regions, the so-called “ray effects” may lead to enhancement of neutron fluxes along the SN angles [2]. For the simplified MSR core, we were not able to successfully within a 2-month period accurately calculate the biological dose rates outside the core where the neutron fluxes are dropped by more than 14 orders of magnitude after passing the thick shielding tank [1].

Because of the significant recent progress made in computer hardware and software development, using the Monte Carlo method to solve the particle transport problem became increasingly popular worldwide. Particularly, leadership facilities with many parallel processors enable simulations to run with billions or trillions of random particles. Variance reduction techniques such as weight windows and source biasing were developed to help drive more random particles toward the interested regions.

In this work, the non-NEAMS Monte Carlo code MCNP6, which has been developed and maintained by LANL for decades, was first applied to solve a simplified MSR ex-core problem [3]. Then, the NEAMS Monte Carlo code Shift, which is being developed at ORNL, was used to model the same problem. Shift is a massively parallel Monte Carlo radiation transport code [4], which made it very attractive for NEAMS to assess its potential use in dose rate and shielding calculations. ANL and ORNL worked together to set up and run the Shift code successfully on the INL HPC cluster. The application of Shift and training of ANL users is the first step towards future work of performing shielding analysis for a more detailed molten salt reactor design such as the Molten Salt Breeder Reactor (MSBR). ANL received significant help from ORNL colleagues within the MSR Application Drivers team to be able to use the code successfully within such a short time.

This report summarizes the assessment work of using both the MCNP code and Shift code for dose rate calculations of the simplified MSR test problem. Section 2 describes the model, Section 3 describes the methodology for both codes, and Section 4 presents and discusses the results.

2 Simplified MSR Model

The simplified MSR model is a graphite moderated molten salt reactor, and it is a direct scale-up of the Molten Salt Reactor Experiment (MSRE) at 500 MWt power. Figure 1 shows a schematic representation of the reactor core, top shield, and water tank. The reactor is below grade so the main region of interest is in position "b" where workers could walk above the water tank. The goal is that with this type of analysis, it is assured that the design has enough water in the tank and the biological dose rates on top of the tank is low enough to allow worker access during normal operations. The model includes a > 2 m borated water layer on top of the core for protection. The half-thickness of water for a Po-Be neutron source (energy of 4 MeV) is about 5.4 cm [5]. If using this parameter, the neutron flux attenuation factor passing the water block can be roughly estimated to ~ 10^{14}.

The detailed geometry and core design are not presented here to avoid potentially disclosing Official Use Only information, but the same geometry and materials were used in both the MCNP and Shift models since Shift accepts MCNP input directly.

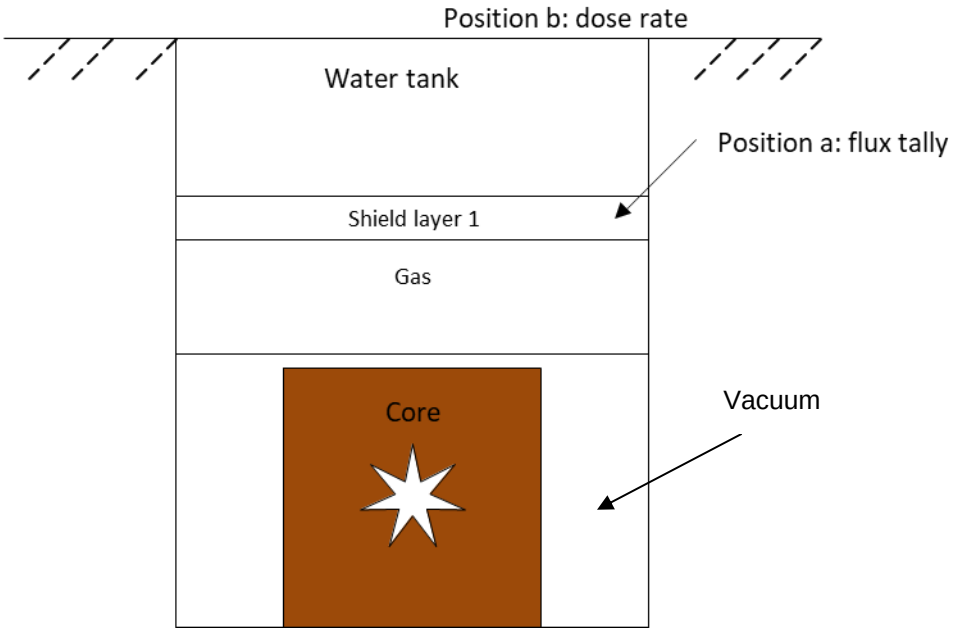


Figure 1 Schematic representation of the simplified MSR model

3 Monte Carlo Methods for Dose Rate Calculations

Unlike the deterministic methods which require discretization of the problem, Monte Carlo methods model the problem continuously in the 3-D geometry space, use continuous particle energy cross section data, and track the particle scattering angle in a continuous 4π space. It uses the pseudo-random number generators to track the particles through a finite number of possible states. The governing probability distributions of each of the possible states are statistically sampled. The results obtained from the Monte Carlo methods are specific tallies which are defined by the users. They are accumulated while following many particle histories and have associated statistical errors. The Monte Carlo method solves the integral particle transport equation which involves no derivative terms in the phase space. It is well suited to solve problems with complicated 3-D geometries [3]. Using Monte Carlo methods, the radiation dose rates can be obtained by tallying the multi-energy group fluxes at positions where user is interested. The standard flux-to-dose-rate conversion factors from the ANSI/ANS-6.1.1-1991 standard can be used to convert the tallied fluxes to the dose rates [6]. Simulations with multiple types of particles coupled or modeled separately, *i.e.*, neutrons and photons, are often performed to calculate the radiation dose rates for nuclear reactor or nuclear facilities. In this initial assessment study, only dose rates from neutrons are calculated.

3.1 Monte Carlo Transport Modes

Typically for nuclear reactors, there are two transport modes to calculate the neutron fluxes: the critical eigenvalue mode and the fixed-source mode. In a critical reactor, the neutron flux distributions are the calculated dominant eigenmode in an eigenvalue calculation since the reactor core is self-sustainable. For a subcritical reactor core, its neutron flux distributions are calculated in a fixed-source mode with the external source specifically modeled. The main difference between the two transport modes in Monte Carlo codes is that in the eigenvalue calculation the neutron particles are tracked generation by generation, while in the fixed-source calculation the neutron particles with all its daughter particles are tracked from their born sites until the particle and its daughter particles all leak out of the system or are absorbed.

For a critical core, the neutron fluxes are calculated by the eigenvalue mode. However, a two-step approach can also be used to obtain the neutron fluxes, with the first step as a nominal eigenvalue calculation to generate the source and the second step as a fixed-source calculation to produce the flux tallies.

In MCNP6, the fission neutrons at their born site can be saved in the first eigenvalue calculation using the SSW card CELL option. Then in the second step, the Monte Carlo transport simulation directly starts from these saved fission neutrons. The fission reaction is turned off to avoid counting those neutrons twice in the second step. Another approach in MCNP6 code is to generate a surface source using the SSW card which records all the particle tracks while passing through user defined surfaces. Then in the second step the transport simulation starts right from the surface where the particle tracks are recorded. Usually in the second step, a reduced geometry model is used to make sure the second transport simulation does not count some of the regions twice. For both approaches, as the transport simulation directly starts with source particles saved from the first step, the tally results obtained from the fixed-source run is automatically normalized to the number of random particles performed in the first eigenvalue calculation.

Shift can also implement a two-step approach to calculate the neutron fluxes in a critical reactor core. The fission source is tallied on a user defined mesh covering the core in the first step eigenvalue calculation. In the second step, the Monte Carlo simulation is continued by sampling the source particles from the spatial distributions defined from the fission mesh tally. The neutron source energies by default are sampled from the ^{235}U Watt spectrum. This is a reasonable assumption for the test model since all fission neutrons are born from ^{235}U fissions if ignoring the ^{238}U fission in the thermal reactor. The fission reaction is turned off in the fixed source calculation. Neutron fluxes are tallied in the second step and its values are normalized to the number of particles run in the second step which is different from the normalization applied in the MCNP6 two-step calculations.

The precision of the calculated neutron fluxes, particularly for the neutron fluxes obtained using the track length tally method is dependent on the number of neutron tracks entering the zone of interest. In nuclear reactors such as the MSR, the positions where the dose rates are evaluated are places away from the core or behind thick shielding materials. For the simplified MSR model, standard analog Monte Carlo simulations showed that it is almost impossible to have any neutron tracks which can penetrate the shielding layer to reach "position b" given a reasonable amount of computer resources. This is due to the expected large neutron flux attenuation in the water tank. Thus, variance reduction techniques needed to be used to achieve sufficient sampling in the zone of interest. Particularly, the two-step approach was adopted to obtain the neutron fluxes at position "b" with the variance techniques applied. The next section will explain why the eigenvalue mode was not used to calculate the neutron fluxes for this test problem.

3.2 Monte Carlo Variance Reduction Techniques

Monte Carlo variance reduction techniques allow the user to improve the computational efficiencies and tally precisions by assigning weight to the particles. This allows more "important particle tracks" to be sampled according to the different particle weights. In the analog Monte Carlo method, all the particles are equally important and have the same weight of 1.0 from creation to removal. In the non-analog Monte Carlo method, the particle weight is adjusted to allow less important particles to be destroyed through Russian Roulette or to enable more important particles to be created through particle splitting. To assure that no bias is introduced to the final tally result, the expected total weight of all particles, which represents the total amount of particles in the problem, is preserved.

Many variance reduction techniques such as forced collision, source biasing, particle splitting, and weight window are implemented in the current Monte Carlo codes. Among them, the weight window is an efficient and popular techniques and is widely used in nuclear reactor applications. The weight window is a phase space with its lower bound usually provided by the user and its upper bound being multiples of the lower bound. When the particle weight is below the weight window, Russian Roulette will be played either to kill the particle or to increase the particle weight within the weight window bounds to allow the particles to continue. When the particle weight is above the weight window, the particle is split to create more particles with their weights adjusted. With the weight window applied in the particle transport simulation, particles will have more chances to be terminated while passing through places assigned with large weights, and will have more chances to be split and create more tracks while passing through places assigned

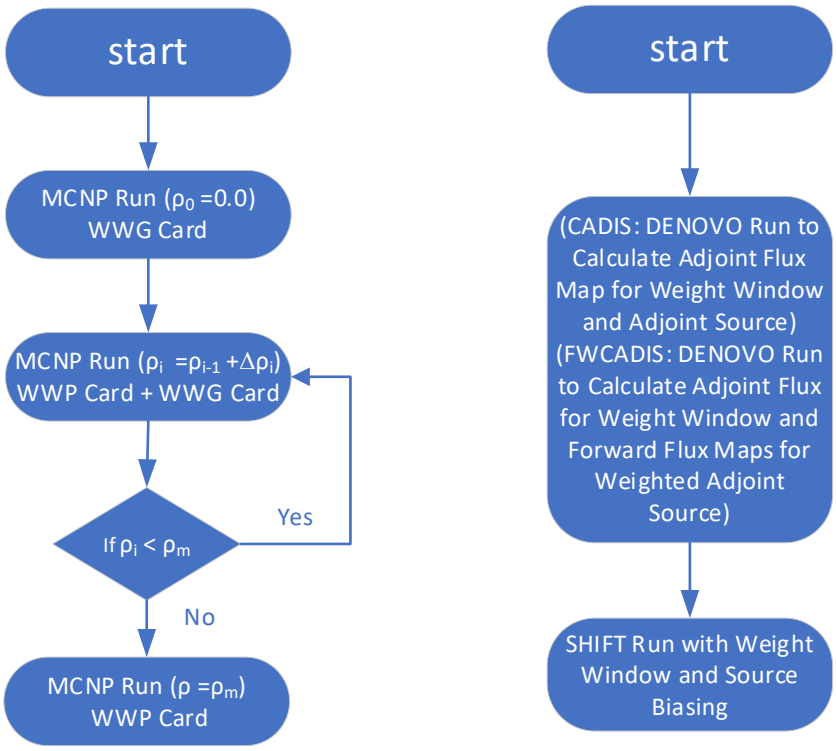
with low weights. Thus, weight windows used in this study are inversely proportional to the particle importance at that position. The weight assigned to different zones in a reactor can be obtained in many ways, and it should not affect or bias the tally results. However, the weight window which is inversely proportional to the particle importance at that position theoretically can lead to almost uniform contributions to the tally for any particle tracks and is proved to be efficient.

In MCNP6, the weight window which is inversely proportional to the particle importance can be obtained using the Weight Window Generator card WWG and with multiple Monte Carlo transport simulations. Figure 2 a) illustrates the iterative process adopted for obtaining the weight window for calculating the simplified MSR problem. It started from a modified Monte Carlo transport simulation in which the material density in the water tank was set to zero or a very small number. During this transport simulation, as no shielding material or only a few percent of the material is placed between position "a" and "b", neutrons are easily transported to position "b" where they are tallied. The WWG card was used in the transport calculation to generate the weight window by tallying the neutron importance on a user specified weight window mesh. In the next step, the Monte Carlo simulations were repeated with increased material density in the water tank. The weight window generated from the previous transport simulation was used to facilitate transporting more particles through the water tank, and a new weight window mesh tally was scored in this step for the next step simulation. The final Monte Carlo transport simulation was performed with the actual water density set in the model, and the weight window generated from its previous step. For the simplified MSR model, three intermediate Monte Carlo transport simulations were performed to generate the weight window with the density in the water tank at about 10%, 20%, and 50% of the nominal value.

The Monte Carlo solver Shift also deploys the weight window technique to become more efficient. This technique is different from that used in MCNP in that it is a "hybrid" method which couples the deterministic method and the Monte Carlo method. Figure 2 b) illustrates the hybrid method used in this study. There are two options in the deterministic step: the Consistent Adjoint Driven Importance Sampling (CADIS) or the Forward-Weighted consistent Adjoint Driven Importance Sampling (FW-CADIS) [4]. With CADIS, the deterministic SN code Denovo, which was developed by ORNL, calculates the adjoint flux (neutron importance) on a simplified and homogenized problem of the original model and generate the weight window for Shift to perform the main transport. The calculated adjoint fluxes also provide a means of consistently biasing the source in the Monte Carlo calculation. With FW-CADIS, Denovo calculates not only the adjoint flux but also the forward flux of the simplified problem. Similar to the CADIS method, the adjoint flux is used to generate the weight window and to bias the source. Furthermore, the biased source will be weighted with the calculated forward flux which will help to reduce the variance if the tallies are global tallies. For the simplified MSR problem, the CADIS and FW-CADIS have about the same efficiencies since the tally of dose rates at position b is only one detector. FW-CADIS was used to produce the results discussed in Section 4.

As mentioned in the previous section, the two-step approach was used instead of the eigenvalue mode to calculate the neutron fluxes away from the core using the variation reduction technique. The reason is because with the weight window technique applied, the weight window usually has large weights inside the reactor core due to their positions far away from the tally position "b". Neutrons will then have large probabilities of being killed while transported inside the core,

where they are born. However, in the eigenvalue calculation, the convergence of the critical eigenvalue k-eff is dependent on the convergence of the fission source within the core. So as more neutrons are killed within the core zone by the weight window, the Monte Carlo calculation of the k-eff will fail to converge. The two-step approach helps avoid this convergence issue. In MCNP6, modifying the weight window in the core zone to have all weights to be zero is another way to get around the convergence issue. However, it is much less efficient than the two-step approach. Therefore, the two-step approach was adopted in both MCNP6 and Shift calculations.



(a) (b)

Figure 2 a) MCNP6 iterative process b) Shift process for calculating the dose rates in the test model.

4 Assessment Results

Three simulations were performed to calculate the dose rates at position "b": A) the simulation was performed using the MCNP6 to generate a fission source file. The fluxes were tallied in the fixed-source calculation coupled with the fission source file. The MCNP6 fixed-source simulation was iterated to generate weight windows in the fixed-source calculation. The weight window was used to push particles into the tally zone in each fixed-source calculations; B) the simulation was performed using MCNP6 to generate a surface source file for neutrons passing through the bottom surface at position "a" towards position "b". The geometry model is then reduced by setting a vacuum boundary at the bottom of the surface where the source is tallied. The fluxes were tallied in the fixed-source calculation coupled with the surface source file on the reduced geometry. The MCNP6 fixed-source simulation was iterated to generate weight windows on the reduced geometry. The weight window was used to facilitate neutrons passing through the water tank to the tally zone; C) the simulation was performed using Shift to generate fission source mesh tallies. The FW-CADIS used Denovo to calculate the weight window. The fluxes were tallied in Shift using the calculated weight window and by sampling the fission source distributions obtained from the fission source mesh tally.

The Shift code has the flexibility to have the geometry model set up in different ways. For the test problem, Shift reads the geometry model from the "runtpe" file generated from the MCNP input. Table 1 first shows the critical eigenvalues of the simplified MSR model calculated by both codes. The eigenvalue k-code calculation without any variance reduction techniques was performed in all these simulations using ENDF/B-7.0 or ENDF/B-7.1 libraries. The Doppler-broadened resonance correction (dbrc) can be turned on and off in Shift and is absent in the MCNP6 simulations. The statistical errors of the calculated k-effs are about 7 pcm for the MCNP6 results and are about 4 pcm for the Shift results. The calculated critical eigenvalues by both codes agreed well with differences around 17 pcm for using the ENDFB7.0 library. The dbrc card only has small impacts on the calculated k-eff. The neutron fluxes at position "a" were also calculated in the k-code calculations, and Table 1 showed very good agreement among the two codes.

Table 1 Calculated k-eff and neutron fluxes at positon "a" for simplified MSR model

	MCNP6		Shift			Δk-eff
	ENDFB-7.0	ENDFB-7.1	ENDFB-7.0 (with dbrc)	ENDFB-7.0 (no dbrc)	ENDFB-7.1 (with dbrc)	ENDFB-7.0 (pcm)
k-eff	1.01613	1.01312	1.01557	1.01596	1.01231	17.0
Flux at position "a" (/source particle)	2.954E-08 (0.15%)	2.948E-08 (0.22%)	2.971E-08 (0.08%)	2.962E-08 (0.08%)	2.964E-09 (0.08%)	----

Table 2 lists the preliminary results obtained at position "b" using MCNP6 and Shift via the three different approaches described earlier. Simulations C1-C4 were performed using the Shift code with slightly different specifications in the Denovo deterministic calculations. Denovo uses the infinite homogeneous medium multigroup cross section data to calculate the adjoint fluxes. For Case C1, the 28 multigroup cross section data collapsed from the ENDF7.0 library were used. For Case C2-C4, the 56 multigroup cross section data were used. The mesh size also varied in the four Denovo calculations. It was around 32 cm in the water tank zone between position "a" and "b" for case C1 and C2, around 12 cm in case C3, and around 5.5 cm in Case C4. We performed the four cases using the different Denovo calculations aiming to better understand how the different specifications in the Denovo calculation may impact the Shift calculations. In these calculations, we have used other default values in the SN calculations, such as the default quadrature and the default number of angles.

The neutron fluxes tallied at position "a" agree with each other among the cases using the same Monte Carlo code (MCNP6 or Shift) but the MCNP6 and Shift results differ by about 13-15% due to the different normalizations implemented for the second-step fixed source calculation. At position "b", the neutron fluxes calculated by the MCNP6 code agree with each other. However, the Shift results showed a large range of variations. The associated statistical errors are large for all of the Shift cases and need to be improved for better comparison in the future investigations. Note that Case A with MCNP6 also had a large statistical error as well. Overall, Table 2 showed that the weight window variance reduction technique has been used successfully to transport neutron particles through the thick shielding layer to reach position "b". As shown in the table, all six cases have predicted that the attenuation factors of the neutron fluxes passing through the water tank is around 5×10^{14}.

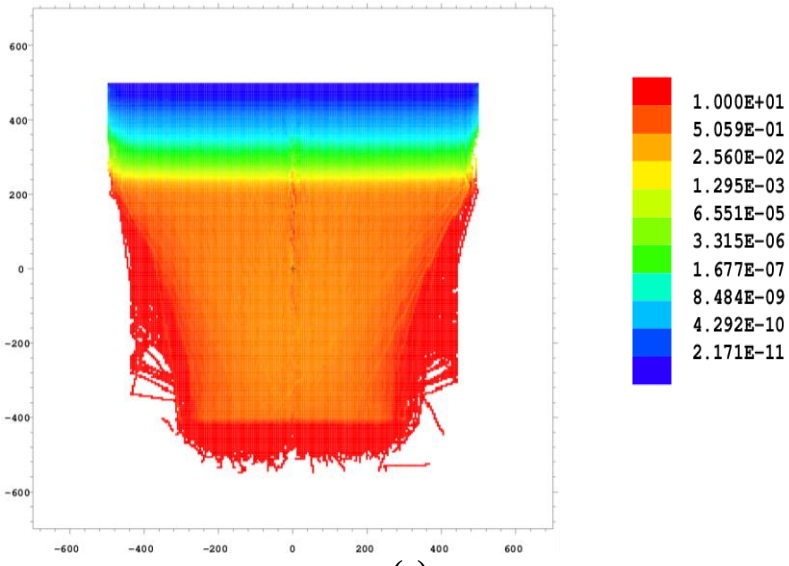
Figure 3 shows the weight windows used in the two MCNP6 simulations (A and B) and Figure 4 shows the adjoint fluxes from Denovo calculation in the Shift C2 case. The weight window should be inversely proportional to the adjoint fluxes shown in Figure 4. In Table 2, Case B has the lowest statistical errors on the calculated neutron fluxes at position "b". As shown in Figure 3, this weight window has the largest flux gradient while crossing the shielding layer. It is also the most effective one among all the cases we tested. Because the transport simulation was performed on the reduced geometry, simulation B also takes the least amount of computational resources. The Case B simulations ran on 63 CPUs on the ANL Eddy2 cluster and finished 1.5E9 source particles by about 45 minutes. The statistical error of the neutron fluxes obtained in simulation A is about twice that in simulation B. The Case A simulation was also run on ANL eddy2 cluster. It used 63 CPUS and finished the 1.5E9 source particles by about 6.5 hours. All the four SHIFT cases C1-C4 were run on the INL HPC cluster taking advantage of the massive amounts of computer cores in the cluster as well as the excellent parallel efficiency of the Shift code. In particular, the simulations C1-C4 deployed 1600 CPUs and finished about 10^{11} particles within about four hours. The current weight window we obtained from the Denovo deterministic calculations are not as effective as the MCNP6 generated. The statistic errors among the four Shift cases are all around 30% or more even though the simulations used almost 60 times more particles than the MCNP cases.

Table 2 Calculated neutron fluxes and dose rates for the simplified MSR model using MCNP6 and Shift with statistical uncertainties in parentheses

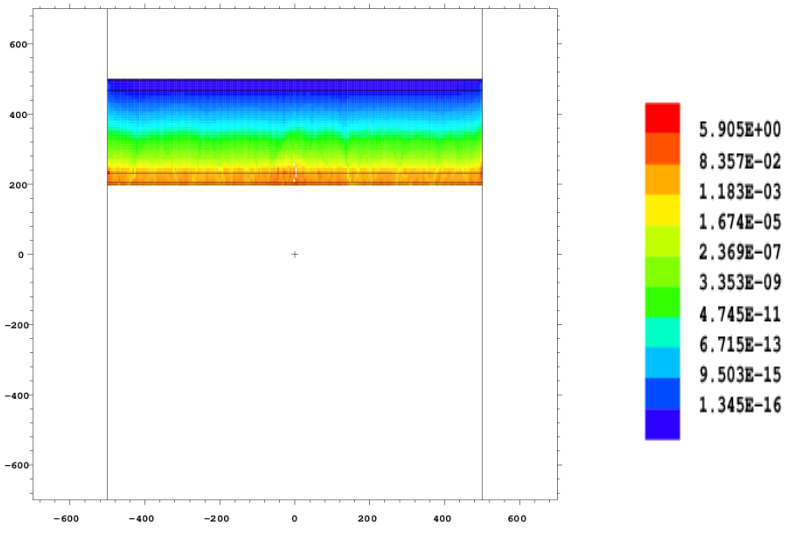
Simulation Cases	Flux at position "a" (/source-particle)	Flux at position "b" (/source-particle)	Flux attenuation factor between position "a" and "b"	Dose Rate at position "b" (mrem/h)
A (MCNP6 fission source file)	2.95E-08 (0.22%)	5.08E-23 (21.4%)	5.81E+14	1.36E-4(23%)
B (MCNP6 surface source file)	2.95E-08 (0.05%)	5.19E-23 (9.97%)	5.68E+14	1.40E-4(10%)
C1 (Shift-28g-32cm)	3.36E-08 (0.007%)	1.53E-22 (30.4%)	2.20E+14	---
C2 (Shift-56g-32cm)	3.36E-08 (0.007%)	6.27E-23 (28.7%)	5.36E+14	---
C3 (Shift-56g-12cm)	3.39E-08 (0.002%)	2.62E-23 (26.2%)	1.29E+15	---
C4 (Shift-56g-5.5cm)	3.39E-08 (0.002%)	2.07E-23 (74.5%)	1.64E+15	---

The actual amount of computer time and user time spent to obtain the weight window is drastically different using the MCNP6 or Shift. For Shift, the weight window generation was part of the overall simulation and its computer time has already been included. The way to set up the Denovo calculation is also straightforward and requires a negligible amount of user effort. For MCNP6, a lot more extra computer time and user effort were spent on generating the weight windows besides the final transport simulation. First of all for simulation B, the way to set up the surface source tally to allow the fixed-source calculation to be performed on a reduced geometry requires the user's intuition and some part of guess work. Reducing the geometry is not always available for all the problems. Second, for both simulations A and B, an iterative process was taken to obtain the weight window. At every iterative step, a full Monte Carlo transport simulation was performed and a similar amount of computer time was required. In addition, there is no guarantee that the iterative procedure can continue for every step. For the test problem for simulation A, the iterative procedure was actually stopped at the case in which 50% of water density was used in the model. The weights in the generated weight window file all suddenly became very large numbers after increasing the water density beyond 50% and are not appropriate for the next step calculation. The reason for the iterative process breaking down might be because the weight window generated from the WWG card is also a mesh tally of the neutron importance and are sensitive to the statistical errors. The weight window presented in Figure 3a was generated with 50% water density placed in the tank and was the one used in the final fixed source calculation in simulation A. Fortunately, the weight window for the test model does not need to be further optimized. In simulation A, the fixed source calculation using this

weight window pushed enough particles through the shield and still provided an estimate of the dose rates at position “b” with reasonable accuracies. An iterative process for generating the weight window for simulation B that involved running cases with 10%, 20%, 30%, 40%, 50%, 65%, 80% and 100% of the nominal water density to obtain the weight window plotted in Figure 3b.



(a)



(b)

Figure 3 a) Weight window for the simulation A using MCNP6 b) Weight window for the simulation B using MCNP6.

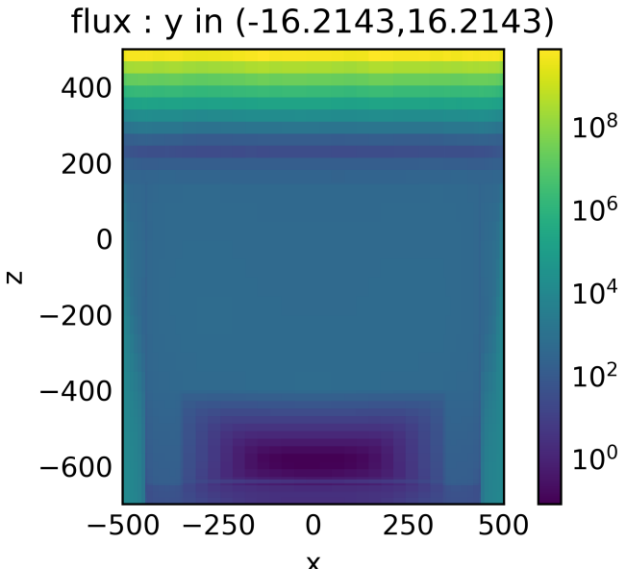


Figure 4 Adjoint flux for the simulation C2 using Shift.

5 Summary

In this work, the Monte Carlo code MCNP6 and the NEAMS Monte Carlo code Shift were tested for their capabilities to calculate radiation dose rates for future MSRs. General procedures of using both codes to solve the deep penetration problem which is often involved in the shielding analysis are discussed. The assessment of both codes was conducted on a simplified MSR model. Our analysis showed that both codes are capable of calculating radiation dose rates at places far away from the core where neutron fluxes are attenuated by more than 10^{14}.

The variance reduction techniques, particularly the weight window, enable both the MCNP6 and Shift codes to transport particles through thick shielding layers. The key differences of generating the weight windows for both codes are discussed in this study. The iterative process of using the MCNP6 code can provide a very efficient weight window but requires user experience and trials of modifying the original numerical model. For some cases, the iterative procedure may break down and a useful weight window is then not guaranteed. The hybrid approach implemented in Shift to calculate the weight window is straightforward and requires less user intervention. Our numerical analysis shows that the weight window efficiencies obtained from the hybrid method may also be dependent on the deterministic solution of the adjoint fluxes and may also need trials to be optimized. However, Shift is very efficient to run on parallel machines and is very easy to be distributed to thousands of CPUs, which allows simulations to be performed even with a slightly less effective weight window but with a larger number of random particles.

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